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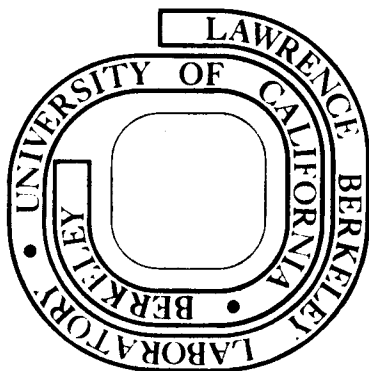
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EMPIRICAL CALCULATIONS OF THE FORCE CONSTANTS,
DISSOCIATION ENERGIES AND BOND LENGTHS OF DIATOMIC MOLECULES*

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ABSTRACT

Empirical equations have been derived to calculate the force constant, F , dissociation energy, D , and bond length, R , of diatomic molecules. They are

$$F_{AX} \cong F_{BX} (F_{A_2}/F_{B_2})^{1/2}$$

$$D_{AX} \cong D_{BX} (D_{A_2}/D_{B_2})^{1/2}$$

and

$$R_{AX} \cong R_{BX} + \frac{1}{2}(R_{A_2} - R_{B_2})$$

where the subscripts stand for atoms A, B, X, Y, respectively. It is also shown that empirical equations in the familiar form

$$F_{AX} \cong F_{BX} (F_{AY}/F_{BY})$$

etc. follow naturally from the above equations.

The use of these equations is illustrated with the existing data on the diatomic alkalis, diatomic halogens and alkali halides. Excellent agreement is obtained for these molecules. The applicabilities of the derived equations to different types of molecules are discussed.

I. INTRODUCTION

The molecular properties such as the force constant, dissociation energy and bond length have long been of interest, both experimentally and theoretically. It often turns out that one needs a simple and reliable estimation of these quantities without having to rigorously solve the quantum mechanics involved. The simplest way would be to find empirical relations which correlate the available data in a simple way with physical significance. Examples are the relations for the force constant by Badger,¹ Guggenheimer,² and Herschbach and Laurie,³ for the bond energy by Pauling,⁴ and for the bond length by Stevenson and Schomaker.⁵

However, an extensive use of these relations is often limited by the following factors. In order to calculate the force constant, one needs to know the bond length of the molecule; to estimate the bond energy and bond length electronegativities of the component atoms in their valence state are needed which are often lacking. It is therefore the purpose of this work to establish some general equations common to these molecular properties and to avoid the limitations inherent in the earlier empirical equations.

In our treatment the concept of electronegativity is retained and yet no explicit values for this quantity are needed in the derived equations. Our idea is to use the existing data on each of the molecular properties and to correlate among the molecules of a certain family of atoms. For example, by correlating the halide of, say, Na with that of K, we would like to estimate the properties of NaX from those of KX; here X could be an alkali atom or other element.

Such an approach has often been adopted, although less explicitly, in estimating the molecular properties. In this work we show how to treat this problem in a more systematic way. In addition, to put this idea one step forward, we would like to estimate NaX from KX by correlating them with Na₂ and K₂. As will be seen later, this latter one is very helpful in finding the molecular quantities for the unknown dimers as well as those for many types of unknown molecules.

Section II shows the derivations of our empirical equations as well as their use which is illustrated with the data on diatomic alkalis, diatomic halogens and alkali halides. The applicabilities to the other types of molecules are discussed in Section III, and the relations of these equations to the earlier ones are discussed in Section IV.

II. METHOD AND CALCULATIONS

Within the framework of the concept of electronegativity we start with the assumption that atom A retains the same electronegativity among molecules AX, AY and AZ; here X, Y and Z belong to the same family which may or may not be the same to that of A. Thus, by correlating molecules AX with AY one would be able to predict the properties of AZ without knowing explicitly the electronegativity of atom A. We first study the force constant and show that the empirical relations developed for this quantity can be well extended to dissociation energy and bond length.

Throughout our treatment in this paper, A, B, C, etc. are elements of the same family, and X, Y, Z, etc. those from another family.

A. Force Constants

The assumption made above states that atom A "behaves the same" toward atoms X, Y and Z in determining the molecular properties, here the force constants F_{AX} , F_{AY} and F_{AZ} . Assuming a product relation, this would require a "constant" contribution of $(F_{A_2}^*)^{1/2}$ from atom A to the force constants of molecules AX, AY and AZ, with the corresponding ones from the atoms X, Y and Z being $(F_{X_2})^{1/2}$, $(F_{Y_2})^{1/2}$ and $(F_{Z_2})^{1/2}$, respectively. Here F_{X_2} is the force constant of molecule X_2 , etc., and $F_{A_2}^*$ is in general different from F_{A_2} , the force constant of molecule A_2 , when atom A is not of the same family as X, Y, Z. Our assumption thus has the form

$$F_{AX} \cong (F_{A_2}^* \times F_{X_2})^{1/2} \quad (A-1)$$

As an example, consider NaCl and NaBr. $F_{Na_2}^*$ is found to be 0.3728 compared with the value of 0.172 m dyne \AA^{-1} for Na_2 .⁶ The higher value for $F_{Na_2}^*$ implies an increasing contribution of Na in going from Na_2 to NaCl and NaBr in determining the force constants of these molecules. This is expected in view of the change in bonding type from Na_2 to the Na halides.

For the molecules composed of atoms from the same family, it is reasonable to assume that atom A has the same contribution in determining the force constants of molecules AB and A_2 . This is similar to assuming that the bonding type is very similar in these molecules. For this type of molecules Eq. (A-1) is thus reduced to

$$F_{AB} \cong (F_{A_2} \times F_{B_2})^{1/2} \quad (A-1')$$

For the alkali and halogen series considered here, Eq. (A-1') holds to within 2% accuracy except for the molecules containing F, which will be discussed later. The force constants of NaCs, KRB and KCs could thus be estimated as 0.110, 0.0897 and 0.0823 m dyne \AA^{-1} , respectively, with an uncertainty of $\pm 2\%$. The data used here are from Jones.⁶

Next, consider molecules AX and AY. From Eq. (A-1) we have

$$F_{AX} \times F_{AY} \cong F_{A_2}^* (F_{X_2} \times F_{Y_2})^{1/2}$$

Applying Eq. (A-1') and rearranging the terms, we have

$$(F_{AX} \times F_{AY})/F_{XY} \cong F_{A_2}^* \quad (1)$$

Similarly, for molecules BX and BY,

$$(F_{BX} \times F_{BY})/F_{XY} \cong F_{B_2}^* \quad (2)$$

Combining Eqs. (1) and (2), we have, for the general form

$$(F_{AX} \times F_{AY})/(F_{BX} \times F_{BY}) \cong F_{A_2}^*/F_{B_2}^* \quad (3)$$

In the special case where X = Y, Eq. (3) becomes

$$F_{AX}/F_{BX} \cong (F_{A_2}^*/F_{B_2}^*)^{1/2} \quad (4)$$

In many cases other than alkali halides, one does not have enough data to find $F_{A_2}^*$, etc. It would therefore be very helpful if one could relate Eq. (4) to F_{A_2} , etc. where data are often available. To do so, we further assume that

$$F_{A_2}^*/F_{B_2}^* \cong F_{A_2}/F_{B_2} \quad (A-2)$$

for A, B being treated toward another family of atoms. In other words, following the earlier assumptions, this is similar to saying that the change in bonding type between A_2 and AX is to the same extent as that between B_2 and BX. Using the available data, we have 1.742 and 1.745 for the ratios F_{Na_2}/F_{K_2} and $F_{Na_2}^*/F_{K_2}^*$, respectively, showing excellent fit with the assumption Eq. (A-2). We thus have our first empirical equation for the force constant

$$F_{AX} \cong F_{BX} (F_{A_2}/F_{B_2})^{1/2} \quad (FC-1)$$

For the cases where values for F_{A_2} and F_{B_2} are not available, a different form of Eq. (FC-1) is needed. From Eq. (FC-1) it holds that

$$F_{AX}/F_{BX} \cong (F_{A_2}/F_{B_2})^{1/2} \cong F_{AY}/F_{BY}$$

which leads to the second empirical equation in the familiar form

$$F_{AX} \cong F_{BX} (F_{AY}/F_{BY}) \quad (\text{FC-2})$$

These are the two empirical equations we will be using to correlate the available data and find the uncertainty limits for the various types of compounds. First, we apply Eq. (FC-1) to the diatomic alkalis and halogens. The results are shown in Table I. Excellent agreement is noted for the available data. Also shown in the Table are the predicted values where data is lacking. It is seen that Eq. (FC-2) also holds very well for these two families, and the calculated values agreed excellently with those using Eq. (FC-1). Take FI for example. Equation (FC-2) gives 3.425 m dyne \AA^{-1} using the observed values of FBr, ClBr and ClI, compared with the value 3.404 m dyne \AA^{-1} calculated from Eq. (FC-1).

Next, both Eq. (FC-1) and Eq. (FC-2) are applied to the alkali halides. This is best seen by finding the F_{MX}/F_{MY} ratios for each of the alkali atoms; here X and Y stand for the halogen atoms. This is shown in Table IIa. Alternatively, we can also find the ratios of $F_{MX}/F_{M'X}$ for each of the halogen atoms; here M and M' stand for the alkali atoms. This is shown in Table IIb.

It is seen that the proportionality constants within each column of Tables IIa and IIb are very nearly the same, thus supporting Eq. (FC-2).

In addition, the constants are close to what one would expect from Eq. (FC-1) except for those cases in Table IIa where fluorine atom is involved. However, Table IIb clearly shows that the fluorides can also be correlated with the other halides through Eq. (FC-1) as well as (FC-2), with the only exception of LiF. Therefore, with proper correlations chosen, both Eq. (FC-1) and Eq. (FC-2) apply very well, and Eq. (FC-1) can be used to provide the proportionality constant wherever necessary.

Applying Eq. (FC-2), the force constants of KI, RbBr, RbI, CsBr and CsI are calculated to be 0.600, 0.624, 0.533, 0.627 and 0.499 m dyne \AA^{-1} , respectively. Here the uncertainties are comparable to that for the other known alkali halides. Alternatively, one could also calculate, say, RbBr from KBr using Eq. (FC-1). The results agree very well with those using Eq. (FC-2).

B. Dissociation Energies

For the dissociation energy we assume that relations similar to those derived for the force constant also apply to this quantity. We have, thus, for the dissociation energy, D , the relations

$$D_{AX} \cong D_{BX} (D_{A_2} / D_{B_2})^{1/2} \quad (\text{DE-1})$$

and

$$D_{AX} \cong D_{BX} (D_{AY} / D_{BY}) \quad (\text{DE-2})$$

with the similar assumption that

$$D_{AB} \cong (D_{A_2} \times D_{B_2})^{1/2} \quad (\text{A-1}')$$

Similar to the force constant work, we first check the validity of Eq. (A-1') which is essential to the validities of Eq. (DE-1) and Eq. (DE-2). The available data⁷ showed excellent agreement with Eq. (A-1') for the diatomic alkalis and halogens, except for the fluorides. Data for the Li-containing diatomic alkalis are not available. However, use is made of the fact that excellent agreement exists among the force constants of LiNa, Li₂ and Na₂. The dissociation energies of the Li-containing diatomic alkalis are thus calculated using Eq. (A-1') and shown in Table III.

Next, Eq. (DE-1) is applied to the diatomic alkalis and the results are shown in Table III. The agreement with the available data is very satisfactory, and the uncertainty limit to be within 5%. Also shown in Table III are the calculations on the diatomic halogens which, too, show good agreement.

Tables IVa and IVb show the results on the alkali halides,⁷ applying Eqs. (DE-1) and (DE-2). Excellent fit with Eq. (DE-2) is noted for all the halides. The proportionality constants are close to the predicted ones from Eq. (DE-1), except for the D_{MF}/D_{MCl} and D_{NaX}/D_{KX} which deviate by factors of about 1.44 and 1.25, respectively, from the values predicted by Eq. (DE-1). It is interesting to note that the former is close to the one of 1.41-1.45 noted for the corresponding one in the force constant case.

C. Bond Lengths

The close dependence of the observed bond length upon the component atomic radii leads us to expect empirical relations for this molecular property similar to those for the force constants and dissociation energies. However, the additivity character of bond lengths implies empirical relations of the form

$$R_{AX} \cong R_{BX} + \frac{1}{2}(R_{A_2} - R_{B_2}) \quad (\text{BL-1})$$

and

$$R_{AX} \cong R_{BX} + (R_{AY} - R_{BY}) \quad (\text{BL-2})$$

with a similar assumption

$$R_{AB} \cong \frac{1}{2}(R_{A_2} + R_{B_2}) \quad (\text{A-1}')$$

Applying Eq. (A-1') to the available data for the diatomic halogens⁸ excellent agreement is obtained for those molecules not containing fluorine atom, as is shown in Table V. Also shown are the calculated bond lengths using Eq. (BL-1) for the diatomic halogens. Calculations on the diatomic alkalis is not done due to the lack of data for the use of Eq. (BL-1). However, success in the force constant and dissociation energy calculations for these molecules lead us to expect that relations Eq. (A-1'), Eq. (BL-1) and Eq. (BL-2) would also hold very well for them.

Next, Eq. (BL-1) and Eq. (BL-2) are applied to the available data on the alkali halides.⁹ The results are shown in Table VI. As expected, Eq. (BL-2) holds very well and the differences are close to the

predicted values from Eq. (BL-1) except for the ($R_{MCI} - R_{MF}$) cases.

Correlations similar to those of Tables IIb and IVb are not given for bond length because of the lack of data for most of the diatomic alkalis.

III. DISCUSSION

It is seen that for the diatomic alkalis and halogens, Eq. (A-1') holds excellently for all the available data except for the fluorine-containing molecules. The agreement is better than those using Eq. (FC-1) and Eq. (FC-2), etc. Therefore, for the molecules not containing fluorine, the calculated values using Eq. (A-1') are preferred. The calculations for these systems using Eq. (FC-1), Eq. (FC-2), etc. are mainly aimed at confirming the validity of these empirical relations before extending our studies to the other inter-family molecules. The very good agreement obtained using the derived relations showed that such a confirmation is satisfactorily accomplished.

The failure of Eq. (A-1') for the fluorine-containing molecules probably implies a rather drastic change in bonding strength between F_2 and FCl , compared with that between Cl_2 and $ClBr$. However, such changes from F_2 to the other fluorides must be very similar among those fluorides, as is reflected by the excellent application of Eq. (FC-2), etc. to these molecules. Furthermore, it is shown that, with suitable choice of correlations, both the halogen fluorides and alkali fluorides can be calculated with Eq. (FC-1), etc. By correlating an unknown fluoride with a known one through Eq. (FC-1), etc., properties of the former can therefore be calculated. As will be seen in a later paper, some of the other second row elements show similarities to fluorine, and molecules containing these elements can be treated in the same way as described here for the fluorides.

It is also worth taking a further look at the empirical relations derived before extending our work to the other series of molecules.

Taking the force constant for example, and the other two properties equally well applicable, Eq. (FC-1) has the form

$$F_{AX} \cong F_{BX} (F_{A_2} / F_{B_2})^{1/2}$$

Here, the central assumption made is that the change in bonding type of atom A between A_2 and AX being the same as that of atom B between B_2 and BX. Thus, this relation should hold best when all A, B, X and Y atoms are in the same valence state. This is the situation for the systems treated in this paper, and excellent fit is obtained with the available data. For a change in valency of atom A between A_2 and AX, and same for atom B, one might encounter larger deviation from that of the system with constant valency. Equation (FC-2) would then be more suitable for these systems. The degree of deviation could vary among different systems and, if possible, one should first check with the available data to find the suitable relations to use in one's calculations.

One advantage of relations Eq. (FC-1), etc. over Eq. (FC-2), etc., respectively, is that one could calculate the properties of molecule A_2 from the available data of molecules containing atom A. The first step is to check the other atoms in atom A's family using Eq. (FC-1), etc. for their applicability to this specific family. The uncertainty limit obtained could then be applied to the calculations of A_2 . Another advantage of the forms Eq. (FC-1), etc. is, as stated earlier, to provide the needed proportionality constants for the calculations of unknown molecules. These facts will be better manifested when we present our calculations on the other series of molecules in the later paper.

IV. CONCLUSIONS

We have derived some empirical relations suitable for the calculations of the force constants, dissociation energies and bond lengths of diatomic molecules. Excellent agreement is obtained for the systems we deal with here.

As was pointed out, the concept of electronegativity is retained in our derivations of the empirical equations, but no explicit values of this quantity are needed for applying these equations. The main contribution of this work is to correlate the molecular properties of a heteronuclear molecule to those of the parent homonuclear ones. This provides a new route and allows estimation of the properties of either type of molecules using the existing data of the other. In addition, the familiar empirical relations often being used, namely Eq. (FC-2), etc., are treated in a more systematic way for fuller uses. Furthermore, a combined use of the present method with the earlier ones would surely lead to a better estimation of those molecular quantities. For example, the estimated bond length from the present method could be used in the earlier empirical methods for the force constant, which, in turn, could be compared with the one obtained from the present method using only the data on the force constants from the relevant molecules.

REFERENCES

- * This work was supported by the U. S. Atomic Energy Commission.
1. R. M. Badger, *J. Chem. Phys.* 2, 128 (1934).
 2. K. M. Guggenheimer, *Proc. Phys. Soc. (London)* 58, 456 (1946).
 3. D. R. Herschbach and V. W. Laurie, *J. Chem. Phys.* 35, 458 (1961).
 4. L. Pauling, *Nature of the Chemical Bond* (Cornell Press, 1960), 3rd ed.
 5. V. Schomaker and D. P. Stevenson, *J. Am. Chem. Soc.* 63, 37 (1941).
 6. L. H. Jones, *Inorganic Vibrational Spectroscopy* (Marcel Dekker, Inc., N. Y., 1971), Vol. 1; data for F_2 from G. DiLorenzo and A. E. Douglas, *J. Chem. Phys.* 56, 5185 (1972). For LiNa: M. M. Hessel, *Phys. Rev. Letters* 26, 215 (1971).
 7. A. G. Gaydon, *Dissociation Energies and Spectra of Diatomic Molecules*, (Chapman and Hall, Ltd., London, 1968), 3rd ed.
 8. *Interatomic Distances* (Chem. Soc. London, 1965).
 9. P. A. Akishin, N. G. Rambidi and V. P. Spiridonov in *The Characterization of High-Temperature Vapors*, J. Margrave, ed. (John Wiley and Sons, Inc., New York, 1967), p. 332.

Table I. Calculated force constants of diatomic alkalis and halogens.

Mol.	F_{obs} m dyne \AA^{-1}	$F_{\text{calc}} (\text{A-1}')$ m dyne \AA^{-1}	$F_{\text{calc}} (\text{FC-1})$ m dyne \AA^{-1}	Remarks*
LiNa	0.208	0.209	0.208	Standard
LiK		0.1585	0.1574	
LiRb		0.1446	0.1436	
LiCs		0.1327	0.1317	
NaK	0.130	0.1302	0.130	Standard
NaRb	0.121	0.1188	0.1186	
NaCs		0.1089	0.1088	
KRb		0.0899	0.0898	
KCs		0.0824	0.0823	
RbCs	0.0748	0.0752	0.0751	
FCl	4.562	3.837	4.705	
FBr	4.071	3.320	4.071	Standard
FI		2.777	3.404	
ClBr	2.832	2.844	2.832	Standard
ClI	2.383	2.378	2.368	
BrI	2.064	2.058	2.049	

* Those marked "standard" are the molecules used to apply Eq. (FC-1). For example, LiNa for LiK, LiRb and LiCs; FBr for FCl and FI; ClBr for ClI and BrI.

Table II. Correlations of the force constants among the alkali halides.

a.				
Atom M	F_{MF}/F_{MCl}	F_{MCl}/F_{MBr}	F_{MBr}/F_{MI}	
Li	1.75	1.18	1.24	
Na	1.60	1.15	1.26	
K	1.59	1.23		
Rb	1.70			
Cs	1.70			
	$(F_{F_2}/F_{Cl_2})^{1/2}=1.17$	$(F_{Cl_2}/F_{Br_2})^{1/2}=1.16$	$(F_{Br_2}/F_{I_2})^{1/2}=1.20$	
b.				
Atom X	F_{LiX}/F_{NaX}	F_{NaX}/F_{KX}	F_{KX}/F_{RbX}	F_{RbX}/F_{CsX}
F	1.41	1.29	1.05	1.07
Cl	1.29	1.27	1.13	1.07
Br	1.26	1.37		
I	1.27			
	$(F_{Li_2}/F_{Na_2})^{1/2}=1.22$	$(F_{Na_2}/F_{K_2})^{1/2}=1.32$	$(F_{K_2}/F_{Rb_2})^{1/2}=1.10$	$(F_{Rb_2}/F_{Cs_2})^{1/2}=1.09$

Table III. Calculated dissociation energies for the diatomic alkalis and halogens.

Mol.	D _{obs} Kcal mol ⁻¹	D _{calc} (A-1') Kcal mol ⁻¹	D _{calc} (DE-1) Kcal mol ⁻¹	Remarks*
LiNa		21.21		
LiK		17.52		
LiRb		16.76		
LiCs		16.44		
NaK	14.3	14.29	13.69	
NaRb	13.1	13.67	13.1	Standard
NaCs		13.41	12.86	
KRb		11.29	10.82	
KCs		11.08	10.62	
RbCs		10.60	10.16	
FCl	59.0	46.0	59.0	Standard
FBr	55.0	41.0	52.6	
FI		36.3	46.6	
ClBr	51.4	50.9	53.1	
ClI	49.63	45.1	47.0	
BrI	41.91	40.2	41.91	Standard

* See footnote of Table I for a similar meaning in applying Eq. (DE-1).

Table IV. Correlations among the dissociation energies of alkali halides.

a.

Atom M	D_{MF}/D_{MCl}	D_{MCl}/D_{MBr}	D_{MBr}/D_{MI}
Li	1.21	1.12	1.22
Na	1.16	1.11	1.25
K	1.16	1.11	1.16
Rb	1.18	1.11	1.15
Cs	1.17	1.12	1.21

$(D_{F_2}/D_{Cl_2})^{1/2}=0.81$ $(D_{Cl_2}/D_{Br_2})^{1/2}=1.12$ $(D_{Br_2}/D_{I_2})^{1/2}=1.13$

b.

Atom X	D_{LiX}/D_{NaX}	D_{NaX}/D_{KX}	D_{KX}/D_{RbX}	D_{RbX}/D_{CsX}
F	1.20	0.98	0.98	0.98
Cl	1.15	0.98	0.99	0.97
Br	1.14	0.97	0.99	0.98
I	1.17	0.90	0.98	1.03

$(D_{Li_2}/D_{Na_2})^{1/2}=1.22$ $(D_{Na_2}/D_{K_2})^{1/2}=1.21$ $(D_{K_2}/D_{Rb_2})^{1/2}=1.05$ $(D_{Rb_2}/D_{Cs_2})^{1/2}=1.02$

Table V. Calculated bond lengths for the diatomic halogens.

Mol.	R_{obs} Å	R_{calc} (A-1') Å	R_{calc} (BL-1) Å	Remarks*
FCl	1.628	1.703	1.6081	
FBr	1.7556	1.851	1.7556	Standard
FI		2.042	1.9471	
ClBr	2.138	2.1358	2.1292	
ClI	2.3208	2.3273	2.3208	Standard
BrI		2.4751	2.4682	

* For example, FBr as the standard in applying Eq. (BL-1) for FCl and FI.

Table VI. Correlations among the bond lengths of the alkali halides.

Atom M	$R_{MCl} - R_{MF}$ Å	$R_{MBr} - R_{MCl}$ Å	$R_{MI} - R_{MBr}$ Å
Li	0.49	0.18	0.19
Na	0.43	0.12	0.23
K	0.50	0.16	0.23
Rb	0.51	0.14	0.20
Cs	0.58	0.17	0.23

$$\frac{1}{2}(R_{Cl_2} - R_{F_2}) = 0.285 \quad \frac{1}{2}(R_{Br_2} - R_{Cl_2}) = 0.1475 \quad \frac{1}{2}(R_{I_2} - R_{Br_2}) = 0.1915$$

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